Individual Differences Multidimensional Scaling

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Abstract

We develop R and C code for Individual Difference Multidimensional Scaling, both for the INDSCAL and the IDIOSCAL case. In addition to the new SMACOF algorithms to minimize the stress loss function we use expressions for the second derivatives with respect to the group configuration and the individual weights to compute perturbation ellipsoids.

Contents

Note: This is a working paper which will be expanded/updated frequently. All suggestions for improvement are welcome. The directory deleeuwpdx.net/pubfolders/stability has a pdf

version, the bib files, the complete Rmd file with the code chunks, and the R and C source code.

1 Introduction

In *Individual Differences Multidimensional Scaling (IDMDS)* we minimize the *stress* loss function, first proposed by Kruskal (1964a), Kruskal (1964b), and defined as

$$\sigma(X_1,\cdots,X_m)=\frac{1}{2}\sum_{k=1}^m\sum\sum_{1\leq i<j\leq n}w_{ijk}(\delta_{ijk}-d_{ij}(X_k))^2 \tag{1}$$

over the $n\times p$ *configurations* $X_1,\cdots,X_m$. In (1) the w_{ijk} are fixed and known *weights*, the δ_{ijk} are fixed and known *dissimilarities*, and $d_{ij}(X_k)$ is the Euclidean distance between rows i and j of X_k.

The configurations are constrained to be of the form$X_k=XT_k$, where T_k is a square matrix of order p. In IDMDS we typically choose T_k to be either a general matrix (IDIOSCAL) or a diagonal matrix (INDSCAL).

2 Weighted Euclidean Distances

The Euclidean distance $d_{ij}(X_k)$ can be expressed in various ways. Some interesting ones, for our purposes, are

$$\begin{aligned}
d_{ij}(X_k)&=\sqrt{(x_i-x_j)'C_k(x_i-x_j)} &(2)\\
&=\sqrt{\mathbf{tr}\ X_k'A_{ij}X_k} &(3)\\
&=\sqrt{x'(C_k\otimes A_{ij})x}, &(4)
\end{aligned}$$

where

$$\begin{aligned}
C_k&=T_kT_k',\\
A_{ij}&=(e_j-e_j)(e_i-e_j)',\\
x_i&=X'e_i,\\
x&=\mathbf{vec}(X).
\end{aligned}$$

In these expressions the e_i and e_j are unit n-element vectors (columns of the identity matrix), with a single element equal to one and all other elements equal to zero. Thus A_{ij} is an $n\times n$ matrix, with elements (i,i) and (j,j) equal to $+1$, elements (i,j) and $j,i)$ equal to -1, and

all other elements equal to zero. We use $\otimes$ for the Kronecker product. The matrix $C_k \otimes A_{ij}$ is a symmetric $np \times np$ matrix, built with the $p \times p$ blocks $c_{kst}A_{ij}$ of size $n \times n$.

Instead of expressing the weighted distance as the square root of a quadratic form in x, we can also find a similar representation as the square root of a quadratic form in the T_k.

$$d_{ij}(X_k) = \sqrt{\mathbf{tr}\ T_k'X'A_{ij}XT_k} = \sqrt{t_k'(I \otimes X'A_{ij}X)t_k} \tag{5}$$

Here $t_k = \mathbf{vec}(T_k)$. The matrix $I \otimes X'A_{ij}X$ is the direct sum of p copies of the $p \times p$ matrix $X'A_{ij}X = (x_i - x_j)(x_i - x_j)'$. If the T_k are diagonal, as in INDSCAL, then we have a more efficient representation.

$$d_{ij}(X_k) = \sqrt{\mathbf{tr}\ T_k'X'A_{ij}XT_k} = \sqrt{t_k'X'A_{ij}Xt_k}, \tag{6}$$

where t_k is now the diagonal of T_k.

3 SMACOF

The basic theory for SMACOF algorithms is in De Leeuw (1977). Applications to IDMDS are in De Leeuw and Heiser (1977) and De Leeuw and Heiser (1980). The IDMDS algorithm suggested in these papers, which is implemented in De Leeuw and Mair (2009), is different from the one we propose in this section.

Let's start by supposing, without loss of generality, that the dissimilarities are normalized, in the sense that

$$\frac{1}{2}\sum_{k=1}^{m}\sum\sum_{1\leq i<j\leq n} w_{ijk}\delta_{ijk}^2 = 1. \tag{7}$$

The IDMDS loss function becomes

$$\sigma(X_1, \cdots, X_m) = 1 - \sum_{k=1}^{m}\sum\sum_{1\leq i<j\leq n} w_{ijk}\delta_{ijk}d_{ij}(X_k) + \frac{1}{2}\sum_{k=1}^{m}\sum\sum_{1\leq i<j\leq n} w_{ijk}d_{ij}^2(X_k). \tag{8}$$

Now

$$\frac{\partial d_{ij}(X_k)}{\partial x} = \frac{1}{d_{ij}(X_k)}(C_k \otimes A_{ij})x, \tag{9}$$

$$\frac{\partial d_{ij}^2(X_k)}{\partial x} = 2(C_k \otimes A_{ij})x, \tag{10}$$

and thus

$$\frac{\partial\sigma(X_1,\cdots,X_m)}{\partial x}=V_\star\,x-B_\star(x)x, \tag{11}$$

where

$$V_\star\;=\sum_{k=1}^m(C_k\otimes V_k), \tag{12}$$

$$B_\star(x)=\sum_{k=1}^m(C_k\otimes B_k(x)), \tag{13}$$

and

$$V_k=\sum\sum_{1\leq i<j\leq n}w_{ijk}A_{ij}, \tag{14}$$

$$B_k(x)=\sum\sum_{1\leq i<j\leq n}w_{ijk}\frac{\delta_{ijk}}{d_{ij}(X_k)}A_{ij}. \tag{15}$$

The SMACOF iterations to minimize (1) over x for given T_k are

$$x^{(\nu+1)}=V_\star^+B_\star(x^{(\nu)})x^{(\nu)}, \tag{16}$$

where ν is the iteration counter and superscript $+$ is the Moore-Penrose inverse.

Now we do the same for the T_k. First the IDIOSCAL case

$$\frac{\partial d_{ij}(X_k)}{\partial t_k}=\frac{1}{d_{ij}(X_k)}(I\otimes X'A_{ij}X)t_k, \tag{17}$$

$$\frac{\partial d_{ij}^2(X_k)}{\partial t_k}=2(I\otimes X'A_{ij}X)t_k, \tag{18}$$

and thus

$$\frac{\partial\sigma(X_1,\cdots,X_m)}{\partial t_k}=(I\otimes X'V_kX)t_k-(I\otimes X'B_k(x)X)t_k. \tag{19}$$

The SMACOF iteration step to update T_k for fixed X is

$$t_k^{(\nu+1)}=(I\otimes(X'V_kX)^+)(I\otimes X'B_k(x)X)t_k^{(\nu)}. \tag{20}$$

Note that this means we can update each column of T_k separately while, of course, we were already updating each T_k separately.

For INDSCAL we have an even simpler iteration on the diagonal of T^k

$$t_k^{(\nu+1)} = (X'V_kX)^+X'B_k(x)Xt_k^{(\nu)}. \tag{21}$$

The overall SMACOF algorithm, implemented in the `smacofIDIOSCAL()` and `smacofINDSCAL()` functions in the appendix, alternates iterations to improve X for fixed T_k with iterations to improve the T_k for fixed X. In our actual implementation we only use a single one of each of these two inner iterations to define a SMACOF step, and after each of these SMACOF steps we test for convergence. Of course the general convergence theory supports algorithms with more than one inner iteration step, but we have not experimented with varying that aspect of the algorithms.

4 Example (Rectangles)

Our example uses data from Borg and Leutner (1983). The data are included in the `smacof` package. In this example $m = 2$, $p = 2$, and $n = 16$. The help file says

> 42 subjects are assigned to two groups of 21 persons. 120 stimulus pairs of rectangles are presented. For the first group (width-height; WH), the rectangles were constructed according to a design as given in rect_constr. For the second group (size-shape; SS) the rectangles were constructed according to a grid design, which is orthogonal in the dimensional system reflecting area (size), and width/height (shape). All subjects had to judge the similarity of the rectangles on a scale from 0 to 9.

The IDIOSCAL and INDSCAL iterations are both started using the output of the `idioscal()` and `indscal()` functions in the `smacof` package as initial configurations. For IDIOSCAL

```
h.idio <- smacofIDIOSCAL (w, delta, res.idio$cweights, res.idio$gspace)
```

```
## itel     1 sold        Inf sa  197.115996 sb    0.070464
## itel     2 sold   0.070464 sa    0.061518 sb    0.060751
## itel     3 sold   0.060751 sa    0.057689 sb    0.057362
## itel     4 sold   0.057362 sa    0.056299 sb    0.056118
## itel     5 sold   0.056118 sa    0.055761 sb    0.055650
## itel     6 sold   0.055650 sa    0.055531 sb    0.055458
## itel     7 sold   0.055458 sa    0.055417 sb    0.055369
## itel     8 sold   0.055369 sa    0.055355 sb    0.055322
## itel     9 sold   0.055322 sa    0.055317 sb    0.055294
## itel    10 sold   0.055294 sa    0.055292 sb    0.055277
## itel    11 sold   0.055277 sa    0.055276 sb    0.055266
## itel    12 sold   0.055266 sa    0.055266 sb    0.055259
## itel    13 sold   0.055259 sa    0.055258 sb    0.055254
```

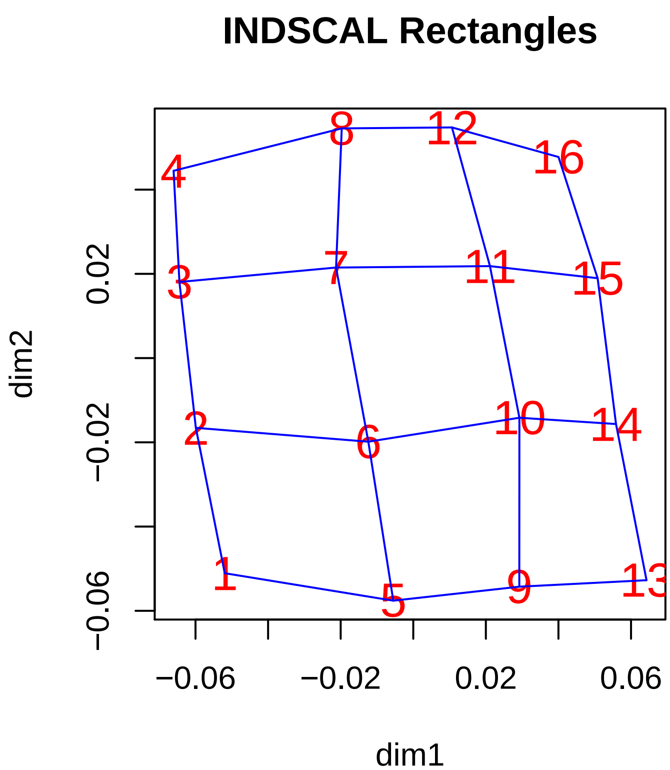
```
## itel    14 sold    0.055254 sa    0.055254 sb    0.055250
## itel    15 sold    0.055250 sa    0.055250 sb    0.055248
## itel    16 sold    0.055248 sa    0.055248 sb    0.055247
## itel    17 sold    0.055247 sa    0.055247 sb    0.055246
## itel    18 sold    0.055246 sa    0.055246 sb    0.055245
```

For INDSCAL the iterations are

```r
h.diag <- smacofINDSCAL (w, delta, res.diag$cweights, res.diag$gspace)
```

```
## itel     1 sold         Inf sa  197.116619 sb    0.070504
## itel     2 sold    0.070504 sa    0.062663 sb    0.061343
## itel     3 sold    0.061343 sa    0.058372 sb    0.057804
## itel     4 sold    0.057804 sa    0.056646 sb    0.056361
## itel     5 sold    0.056361 sa    0.055928 sb    0.055770
## itel     6 sold    0.055770 sa    0.055611 sb    0.055517
## itel     7 sold    0.055517 sa    0.055459 sb    0.055399
## itel     8 sold    0.055399 sa    0.055378 sb    0.055339
## itel     9 sold    0.055339 sa    0.055331 sb    0.055305
## itel    10 sold    0.055305 sa    0.055302 sb    0.055284
## itel    11 sold    0.055284 sa    0.055283 sb    0.055271
## itel    12 sold    0.055271 sa    0.055271 sb    0.055262
## itel    13 sold    0.055262 sa    0.055262 sb    0.055257
## itel    14 sold    0.055257 sa    0.055257 sb    0.055253
## itel    15 sold    0.055253 sa    0.055253 sb    0.055250
## itel    16 sold    0.055250 sa    0.055250 sb    0.055248
## itel    17 sold    0.055248 sa    0.055248 sb    0.055247
## itel    18 sold    0.055247 sa    0.055247 sb    0.055246
```

As the minimum of the stress already suggests the two solutions for X are basically indistinguishable. We plot the one from INDSCAL.



Since there are only two different distance matrices we do not plot the T_k. For IDIOSCAL they are

```
## [[1]]
##                D1            D2
## D1  0.9969528775 -0.1401381035
## D2 -0.1900447368  1.0747955535
##
## [[2]]
##              D1           D2
## D1 1.0810614200 0.1374772239
## D2 0.1829126197 0.8261765584
```

and for INDSCAL we have

```
## [[1]]
##              [,1]        [,2]
## [1,] 0.8760383307 0.000000000
## [2,] 0.0000000000 1.312868518
##
## [[2]]
##             [,1]         [,2]
## [1,] 1.162505002 0.0000000000
## [2,] 0.000000000 0.8206214109
```

The T_k from IDIOSCAL are hevily diagonally dominant, which explains why INDSCAL and

IDIOSCAL are very similar.

5 Example (Colors)

Our second, somewhat larger, example uses data from Helm (1959), also included in the smacof package. From the help file:

> A detailed description of the experiment can be found in Borg and Groenen (2005), p. 451 with the corresponding Table 21.1. containing distance estimates for color pairs. There were 14 subjects that rated the similarity of colors, 2 of whom replicated the experiment. 10 subjects have a normal color vision (labelled by N1 to N10 in our list object), 4 of them are red-green deficient in varying degrees. In this dataset we give the dissimilarity matrices for each of the subjects, including the replications.

The IDIOSCAL iterations are:

```
h.idio <- smacofIDIOSCAL (weights, delta, idi.helm$cweights, idi.helm$gspace)
```

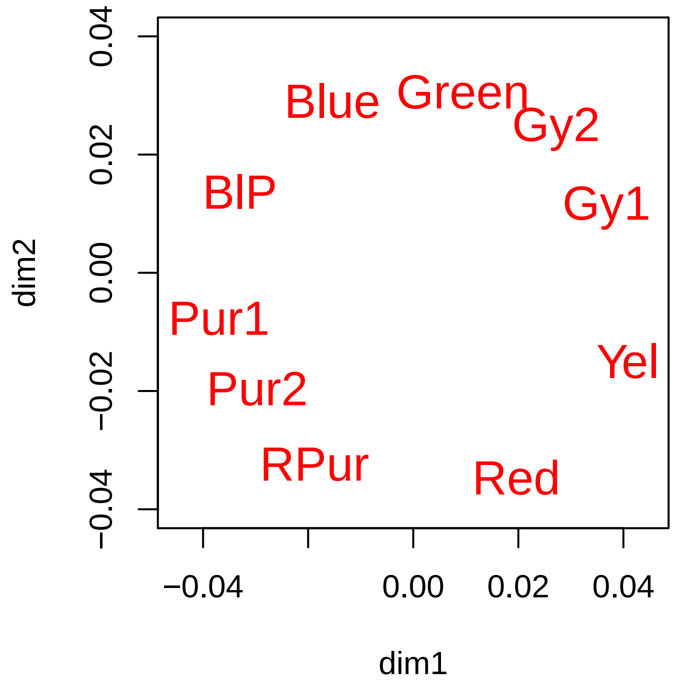
```
## itel     1 sold        Inf sa  632.304054 sb    0.063500
## itel     2 sold   0.063500 sa    0.043978 sb    0.043829
## itel     3 sold   0.043829 sa    0.043316 sb    0.043283
## itel     4 sold   0.043283 sa    0.043092 sb    0.043083
## itel     5 sold   0.043083 sa    0.043015 sb    0.043013
## itel     6 sold   0.043013 sa    0.042989 sb    0.042988
## itel     7 sold   0.042988 sa    0.042980 sb    0.042980
## itel     8 sold   0.042980 sa    0.042977 sb    0.042977
## itel     9 sold   0.042977 sa    0.042976 sb    0.042976
```

The INDSCAL iterations are:

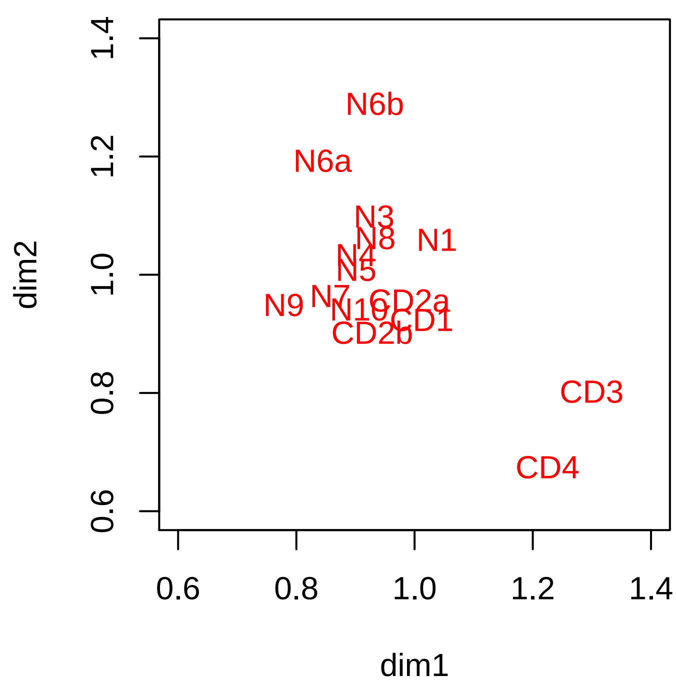
```
h.diag <- smacofINDSCAL (weights, delta, ind.helm$cweights, ind.helm$gspace)
```

```
## itel     1 sold        Inf sa  631.986429 sb    0.065305
## itel     2 sold   0.065305 sa    0.046937 sb    0.046808
## itel     3 sold   0.046808 sa    0.046355 sb    0.046325
## itel     4 sold   0.046325 sa    0.046131 sb    0.046123
## itel     5 sold   0.046123 sa    0.046037 sb    0.046035
## itel     6 sold   0.046035 sa    0.045995 sb    0.045993
## itel     7 sold   0.045993 sa    0.045974 sb    0.045973
## itel     8 sold   0.045973 sa    0.045963 sb    0.045962
## itel     9 sold   0.045962 sa    0.045956 sb    0.045956
## itel    10 sold   0.045956 sa    0.045953 sb    0.045952
## itel    11 sold   0.045952 sa    0.045951 sb    0.045950
## itel    12 sold   0.045950 sa    0.045949 sb    0.045949
## itel    13 sold   0.045949 sa    0.045948 sb    0.045948
```

INDSCAL Helm Configuration



INDSCAL Helm Weights



6 Stability

In this paper we study, in addition, the stability of IDMDS solutions. We define stability in the usual way. In inferential statistics we look at the second derivatives of the likelihood function at the maximum likelihood estimate. In MDS we look at the second derivatives of stress at a local minimum. Our results extend the results in De Leeuw (2017) from MDS to IDMDS.

In general, if a function $f:\mathbb{R}^n \Rightarrow \mathbb{R}$ is two times continuously differentiable then

$$f(x) = f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'\mathcal{D}^2f(y)(x-y) + o(\|x-y\|).$$

If f has a local minimum in y then $\mathcal{D}f(y) = 0$ and $\mathcal{D}^2f(y) \gtrsim 0$. Consider all x of the form

$$x = \begin{bmatrix} x_1 \\ y_2 \end{bmatrix}, \tag{22}$$

where y_2 has the last $n-m$ elements of y. Then

$$f(x) = f(y) + \frac{1}{2}(x_1-y_1)'H(y)(x_1-y_1) + o(\|x_1-y_1\|), \tag{23}$$

where $H(y)$ is the leading $m\times m$ submatrix of the $\mathcal{D}^2f(y)$. Thus the set of all x of the form (22) with $f(x) \leq (1+\epsilon)f(y)$ can be approximated by choosing x_1 in the ellipsoid

$$(x_1-y_1)'H(y)(x_1-y_1) \leq 2\epsilon f(y) \tag{24}$$

We could choose ϵ to be 0.1, for example, which means we look at a perturbation region where stress is at most 10% larger than the minimum we have found.

To apply these general results to IDMDS we need the second derivatives of stress. Of course these second derivatives can also be used for other purposes, such as checking the necessary conditions for a local minimum, or for implementations of Newton's method. Start with the derivatives with repect to X. We have

$$\frac{\partial^2 d_{ij}(X_k)}{\partial x\partial x} = \frac{1}{d_{ij}(X_k)}\left\{(C_k\otimes A_{ij}) - \frac{(C_k\otimes A_{ij})xx'(C_k\otimes A_{ij})}{d_{ij}^2(X_k)}\right\}, \tag{25}$$

and, of course,

$$\frac{\partial^2 d_{ij}^2(X_k)}{\partial x\partial x} = C_k\otimes A_{ij}. \tag{26}$$

Thus

$$\frac{\partial^2\sigma(X_1,\cdots,X_m)}{\partial x\partial x}=V_\star-H_\star(x),\tag{27}$$

where

$$H_\star(x)=\sum_{k=1}^m\sum\sum_{1\le i<j\le n}w_{ijk}\frac{\delta_{ijk}}{d_{ij}(X_k)}\left\{(C_k\otimes A_{ij})-\frac{(C_k\otimes A_{ij})xx'(C_k\otimes A_{ij})}{d_{ij}^2(X_k)}\right\}.\tag{28}$$

We now look at the second derivatives with repect to the T_k. First the IDIOSCAL case, which has

$$\frac{\partial^2 d_{ij}^2(X_k)}{\partial t_k\partial t}=I\otimes X'A_{ij}X,\tag{29}$$

and

$$\frac{\partial^2 d_{ij}(X_k)}{\partial t_k\partial t_k}=\frac{1}{d_{ij}(X_k)}\left\{(I\otimes X'A_{ij}X)-\frac{(I\otimes X'A_{ij}X)t_kt_k'(I\otimes X'A_{ij}X)}{d_{ij}^2(X_k)}\right\}.\tag{30}$$

$$\frac{\partial^2\sigma(X_1,\cdots,X_m)}{\partial t_k\partial t_k}=(I\otimes X'V_kX)-G_k(t_k),\tag{31}$$

where

$$G_k(t_k)=\sum\sum_{1\le i<j\le n}w_{ijk}\frac{\delta_{ijk}}{d_{ij}(X_k)}\left\{(I\otimes X'A_{ij}X)-\frac{(I\otimes X'A_{ij}X)t_kt_k'(I\otimes X'A_{ij}X)}{d_{ij}^2(X_k)}\right\}.\tag{32}$$

For the INDSCAL case we have the same formulas, but without the $I\otimes$ part. Thus

$$\frac{\partial^2\sigma(X_1,\cdots,X_m)}{\partial t_k\partial t_k}=X'V_kX-G_k(t_k),\tag{33}$$

where

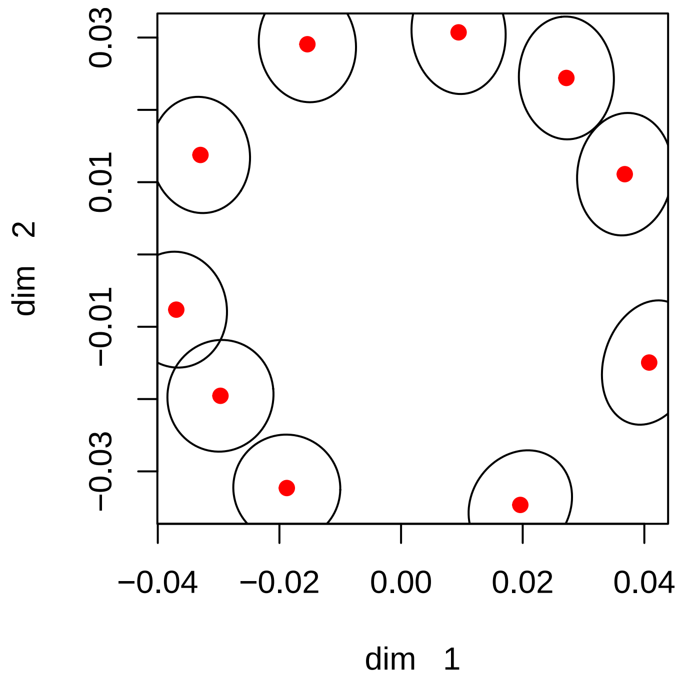
$$G_k(t_k)=\sum\sum_{1\le i<j\le n}w_{ijk}\frac{\delta_{ijk}}{d_{ij}(X_k)}\left\{X'A_{ij}X-\frac{X'A_{ij}Xt_kt_k'X'A_{ij}X}{d_{ij}^2(X_k)}\right\}.\tag{34}$$

We should perhaps mention that the perturbation results for IDIOSCAL are limited by the fact that the representation of X_k as XT_k is far from unique. Besides the obvious, and rather harmless, unidentifiability due to translation and expansion, we also have $XT_k=(XQ)(Q^{-1}T_k)$ for any nonsingular Q. This suggests we should incorporate an identification condition such as $T_1=I$ in our equations. We haven't done this yet. Until we have chosen the identification condition the stability analysis for IDIOSCAL is not yet available. Note that the identification condition is not needed for the SMACOF algorithm, but it is needed for the stability analysis.

7 Example (Colours Stability)

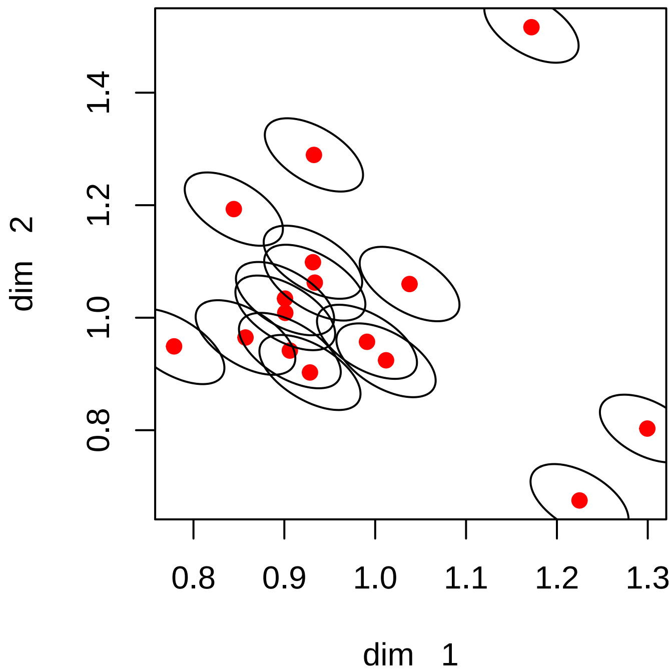
We now apply our second derivative information to the Helm INDSCAL analysis. First for the configuration X.

```
par(pty="s")
hh<-smacofDerivativesX (weights, delta, h.diag$b, h.diag$x)
smacofEllipsesX (h.diag$x, hh$h, hh$s, .05, 1, 2)
```



For the weights T_k in INDSCAL we compute a separate 2×2 matrix of derivatives for each of the 16 replications.

```
bbb <- t(sapply (h.diag$b, diag))
hh <- array (0, c(2, 2, 16))
for (k in 1:16) {
  hk<-smacofDerivativesTKDiag (weights[[k]], delta[[k]], h.diag$b[[k]], h.diag$x)
  hh[, , k] <- hk$h
}
smacofEllipsesTDiag (bbb, hh, h.diag$s, .002, 1, 2)
```



It is remarkable that both the orientation and size of the ellipses are basically the same over the 16 replications. It remains to be seen if this is specific to this example or if it happens more generally.

8 Projection

In our stability analysis for X we change row x_i, and we keep all other rows and all T_k fixed and constant. As an alternative we could look at

$$\sigma_\bullet(X) = \min_{T_1,\cdots,T_k} \sigma(X_1,\cdots,X_k). \tag{35}$$

We project out the T_k and loss becomes a function of X only. Now

$$\frac{\partial^2\sigma_\bullet(X)}{\partial x\partial x} = \frac{\partial^2\sigma(X_1,\cdots,X_k)}{\partial x\partial x} - \sum_{k=1}^m \frac{\partial^2\sigma(X_1,\cdots,X_k)}{\partial x\partial t_k}\left[\frac{\partial^2\sigma(X_1,\cdots,X_k)}{\partial t_k\partial t_k}\right]^+ \frac{\partial^2\sigma(X_1,\cdots,X_k)}{\partial t_k\partial x}. \tag{36}$$

We have not implemented this alternative defintion of stability yet, mainly because it requires in addition the mixed second partials with respect to x and the t_k. Clearly at a minimum

$$\frac{\partial^2\sigma_\bullet(X)}{\partial x\partial x} \lesssim \frac{\partial^2\sigma(X_1,\cdots,X_k)}{\partial x\partial x}, \tag{37}$$

which implies the perturbation ellipsoids will be larger.

9 Nonmetric MDS

In our results so far we have treated the δ_{ijk} as fixed constants. In Nonmetric Multidimensional Scaling (NMDS), however, stress can be defined as

$$\sigma(X_1,\cdots,X_m)=\frac{1}{2}\sum_{k=1}^m\min_{\delta_k\in\Delta_k}\sum_{1\leq i<j\leq n}\sum w_{ijk}(\delta_{ijk}-d_{ij}(X_k))^2, \tag{38}$$

which makes the dissimilarities a function of the X_k. This projection changes the perturbation results for the X_k, in the same way as the result in the previous section did. But with NMDS there is an additional complication. Typically the dissimilarities are minimized over the polyhedral cones that define monotone regression. Although the partial minimum of stress over the cone is differentiable with respect to the X_k, it is not twice differentiable, because the monotone regression transformation itself is not differentiable. Again, we have chosen not to implement the resulting complications (yet).

The perturbation results we have can be applied in NMDS, but the perturbation regions must be interpreted in terms of moving the points in the configuration for a given set of dissimilarties, which can of course be the optimal dissimilarities computed by NMDS.

10 Appendix: Code

10.1 smacofIDIOSCAL.R

```
# w is list of length m with n x n matrices
# delta is list of length m with  n x n matrices
# b is list of length m with  p x p matrices
# x is n x p

smacofIDIOSCAL <-
  function (w,
            delta,
            b,
            x,
            itmax = 100,
            eps = 1e-6,
            verbose = TRUE) {
    n <- nrow (x)
    p <- ncol (x)
    m <- length (w)
    itel <- 1
    sold <- Inf
    repeat {
      sa <- 0.0
```

```
    v <- matrix (0, n * p, n * p)
    u <- matrix (0, n * p, n * p)
    for (k in 1:m) {
      cmat <- tcrossprod (b[[k]])
      xmat <- x %*% b[[k]]
      dmat <- as.matrix (dist (xmat))
      vmat <- -w[[k]]
      diag(vmat) <- -rowSums(vmat)
      bmat <- -delta[[k]] * ifelse (dmat == 0, 0, 1 / dmat)
      diag(bmat) <- -rowSums(bmat)
      sa <-
        sa + sum (w[[k]] * (delta[[k]] - dmat) ^ 2) / 2.0
      v <- v + kronecker (cmat, vmat)
      u <- u + kronecker (cmat, bmat)
    }
    x <- matrix (ginv (v) %*% u %*% as.vector (x), n, p)
    sb <- 0.0
    for (k in 1:m) {
      xmat <- x %*% b[[k]]
      dmat <- as.matrix (dist (xmat))
      vmat <- -w[[k]]
      diag(vmat) <- -rowSums(vmat)
      hmat <- crossprod (x, vmat %*% x)
      bmat <- -delta[[k]] * ifelse (dmat == 0, 0, 1 / dmat)
      diag(bmat) <- -rowSums(bmat)
      gmat <- crossprod (x, bmat %*% x)
      sb <-
        sb + sum (w[[k]] * (delta[[k]] - dmat) ^ 2) / 2.0
      kmat <- ginv (hmat) %*% gmat
      for (j in 1:p) {
        b[[k]][, j] <- kmat %*% b[[k]][, j]
      }
    }
    if (verbose) {
      cat(
        "itel ",
        formatC (itel, digits = 3, format = "d"),
        "sold ",
        formatC (
          sold,
          digits = 6,
          width = 10,
          format = "f"
        ),
```

```
          "sa ",
          formatC (
            sa,
            digits = 6,
            width = 10,
            format = "f"
          ),
          "sb ",
          formatC (
            sb,
            digits = 6,
            width = 10,
            format = "f"
          ),
          "\n"
        )
      }
      if ((itel == itmax) || (sold - sb < eps))
        break
      sold <- sb
      itel <- itel + 1
    }
    return (list (x = x, b = b, s = sb))
  }
```

10.2 smacofINDSCAL.R

```
# w is list of length m with n x n matrices
# delta is list of length m with  n x n matrices
# b is list of length m with  p x p matrices
# x is n x p

smacofINDSCAL <- function (w, delta, b, x, itmax = 100, eps = 1e-6, verbose = TRUE) {
  n <- nrow (x)
  p <- ncol (x)
  m <- length (w)
  itel <- 1
  sold <- Inf
  repeat {
    sa <- 0.0
    v <- matrix (0, n * p, n * p)
    u <- matrix (0, n * p, n * p)
    for (k in 1:m) {
      cmat <- tcrossprod (b[[k]])
```

```
    xmat <- x %*% b[[k]]
    dmat <- as.matrix (dist (xmat))
    vmat <- -w[[k]]
    diag(vmat) <- -rowSums(vmat)
    bmat <- -delta[[k]] * ifelse (dmat == 0, 0, 1 / dmat)
    diag(bmat) <- -rowSums(bmat)
    sa <-
      sa + sum (w[[k]] * (delta[[k]] - dmat) ^ 2) / 2.0
    v <- v + kronecker (cmat, vmat)
    u <- u + kronecker (cmat, bmat)
  }
  x <- matrix (ginv (v) %*% u %*% as.vector (x), n, p)
  sb <- 0.0
  for (k in 1:m) {
    xmat <- x %*% b[[k]]
    dmat <- as.matrix (dist (xmat))
    vmat <- -w[[k]]
    diag(vmat) <- -rowSums(vmat)
    hmat <- crossprod (x, vmat %*% x)
    bmat <- -delta[[k]] * ifelse (dmat == 0, 0, 1 / dmat)
    diag(bmat) <- -rowSums(bmat)
    gmat <- crossprod (x, bmat %*% x)
    sb <-
      sb + sum (w[[k]] * (delta[[k]] - dmat) ^ 2) / 2.0
    kmat <- ginv (hmat) %*% gmat
    b[[k]] <- diag (drop (kmat %*% diag (b[[k]])))
  }
  if (verbose) {
    cat(
      "itel ",
      formatC (itel, digits = 3, format = "d"),
      "sold ",
      formatC (
        sold,
        digits = 6,
        width = 10,
        format = "f"
      ),
      "sa ",
      formatC (
        sa,
        digits = 6,
        width = 10,
        format = "f"
```

```
        ),
        "sb ",
        formatC (
          sb,
          digits = 6,
          width = 10,
          format = "f"
        ),
        "\n"
      )
    }
    if ((itel == itmax) || (sold - sb < eps))
      break
    sold <- sb
    itel <- itel + 1
  }
  return (list (x = x, b = b, s = sb))
}
```

10.3 smacofDerivatives.R

```
smacofDerivativesX <- function (w, delta, b, x) {
  n <- nrow (x)
  p <- ncol (x)
  m <- length (w)
  s <- 0.0
  v <- matrix (0, n * p, n * p)
  u <- matrix (0, n * p, n * p)
  r <- matrix (0, n * p, n * p)
  for (k in 1:m) {
    cmat <- tcrossprod (b[[k]])
    xmat <- x %*% b[[k]]
    dmat <- as.matrix (dist (xmat))
    for (i in 1:(n - 1)) {
      for (j in (i + 1):n) {
        ei <- ifelse (i == 1:n, 1, 0)
        ej <- ifelse (j == 1:n, 1, 0)
        amat <- outer (ei - ej, ei - ej)
        kmat <- kronecker (cmat, amat)
        kx <- drop (kmat %*% as.vector(x))
        kxkx <- outer (kx, kx)
        s <- s + w[[k]][i, j] * (delta[[k]][i, j] - dmat [i, j]) ^ 2
        v <- v + w[[k]][i, j] * kmat
```

```
        u <-
          u + w[[k]][i, j] * (delta[[k]][i, j] / dmat[i, j]) * kmat
        r <-
          r + w[[k]][i, j] * (delta[[k]][i, j] / (dmat [i, j] ^ 3)) * kxkx
      }
    }
  }
  g <- drop ((v - u) %*% as.vector(x))
  h <- v - u + r
  return (list (s = s, g = 0, h = h))
}

smacofDerivativesTKDiag <- function (w, delta, b, x) {
  n <- nrow (x)
  p <- ncol (x)
  s <- 0.0
  v <- matrix (0, p, p)
  u <- matrix (0, p, p)
  r <- matrix (0, p, p)
  cmat <- tcrossprod (b)
  xmat <- x %*% b
  dmat <- as.matrix (dist (xmat))
  for (i in 1:(n - 1)) {
    for (j in (i + 1):n) {
      ei <- ifelse (i == 1:n, 1, 0)
      ej <- ifelse (j == 1:n, 1, 0)
      amat <- outer (ei - ej, ei - ej)
      kmat <- crossprod(x, amat %*% x)
      kx <- drop (kmat %*% diag(b))
      kxkx <- outer (kx, kx)
      s <- s + w[i, j] * (delta[i, j] - dmat [i, j]) ^ 2
      v <- v + w[i, j] * kmat
      u <-
        u + w[i, j] * (delta[i, j] / dmat[i, j]) * kmat
      r <-
        r + w[i, j] * (delta[i, j] / (dmat[i, j] ^ 3)) * kxkx
    }
  }
  g <- drop ((v - u) %*% diag(b))
  h <- v - u + r
  return (list (s = s, g = g, h = h))
}

smacofDerivativesTKFull <- function (w, delta, b, x) {
```

```
  n <- nrow (x)
  p <- ncol (x)
  m <- length (w)
  s <- 0.0
  v <- matrix (0, n * p, n * p)
  u <- matrix (0, n * p, n * p)
  r <- matrix (0, n * p, n * p)
  cmat <- tcrossprod (b[[k]])
  xmat <- x %*% b[[k]]
  dmat <- as.matrix (dist (xmat))
  for (i in 1:(n - 1)) {
    for (j in (i + 1):n) {
      ei <- ifelse (i == 1:n, 1, 0)
      ej <- ifelse (j == 1:n, 1, 0)
      amat <- outer (ei - ej, ei - ej)
      kmat <- kronecker (cmat, amat)
      kx <- drop (kmat %*% diag(x))
      s <- s + w[[k]][i, j] * (delta[[k]][i, j] - dmat [i, j]) ^ 2
      v <- v + w[[k]][i, j] * kmat
      u <-
        u + w[[k]][i, j] * (delta[[k]][i, j] / dmat[i, j]) * kmat
      r <-
        r + w[[k]][i, j] * (delta[[k]][i, j] / dmat[i, j]) * (outer (kx, kx) / (dmat [i,
    }
  }
  g <- drop ((v - u) %*% as.vector(x))
  h <- v - u + r
  return (list (s = s, g = g, h = h))
}
```

10.4 smacofEllipses.R

```
smacofEllipsesX <- function (x, h, f, eps, s = 1, t = 2) {
  n <- nrow (x)
  plot (
    x,
    col = "RED",
    pch = 21,
    bg = "RED",
    xlab = paste("dim ", formatC(
      s, digits = 1, format = "d"
    )),
    ylab = paste("dim ", formatC(
```

```
      t, digits = 1, format = "d"
    ))
  )
  z <-
    cbind (sin (seq(-pi, pi, length = 100)),
           cos (seq(-pi, pi, length = 100))) * sqrt(2 * eps * f)
  for (i in 1:n) {
    ii <- c((s - 1) * n + i, (t - 1) * n + i)
    y <- x[i, c(s, t)]
    amat <- h[ii, ii]
    heig <- eigen (amat)
    zi <- z %*% diag (1 / sqrt (heig$values))
    zi <- tcrossprod(zi, heig$vectors)
    zi <- zi + matrix (y, 100, 2, byrow = TRUE)
    lines (list(x = zi[, 1], y = zi[, 2]))
  }
}

smacofEllipsesTDiag <- function (b, h, f, eps, s = 1, t = 2) {
  par (pty= "s")
  m <- nrow (b)
  ii <- c(s, t)
  plot (
    b[, ii],
    col = "RED",
    pch = 21,
    bg = "RED",
    xlab = paste("dim ", formatC(
      s, digits = 1, format = "d"
    )),
    ylab = paste("dim ", formatC(
      t, digits = 1, format = "d"
    ))
  )
  z <-
    cbind (sin (seq(-pi, pi, length = 100)),
           cos (seq(-pi, pi, length = 100))) * sqrt(2 * eps * f)
  for (k in 1:m) {
    y <- b[k, ii]
    amat <- h[ii, ii, k]
    heig <- eigen (amat)
    zi <- z %*% diag (1 / sqrt (heig$values))
    zi <- tcrossprod(zi, heig$vectors)
    zi <- zi + matrix (y, 100, 2, byrow = TRUE)
```

```
    lines (list(x = zi[, 1], y = zi[, 2]))
  }
}
```

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